5,5-Bis[(^{2}H$_3$)methyl]-3-[4-nitro-3-(trifluoromethyl)phenyl]imidazolidine-2,4-dione

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.02e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.31e-01

Confidence level: 3.99e-01

Nearest Neighbors from the Training Set

Image not found
Bentazone
Measured: 2.08e-03
Predicted: 4.04e-03

Image not found
Endosulfan sulfate
Measured: 1.14e-06
Predicted: 6.86e-06

Image not found
Cyclobutanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 1.00e-03
Predicted: 3.91e-04

Image not found
Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-,
methyl ester
Measured: 4.91e-04
Predicted: 9.14e-04

Image not found
Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 2.88e-04
Predicted: 2.63e-04